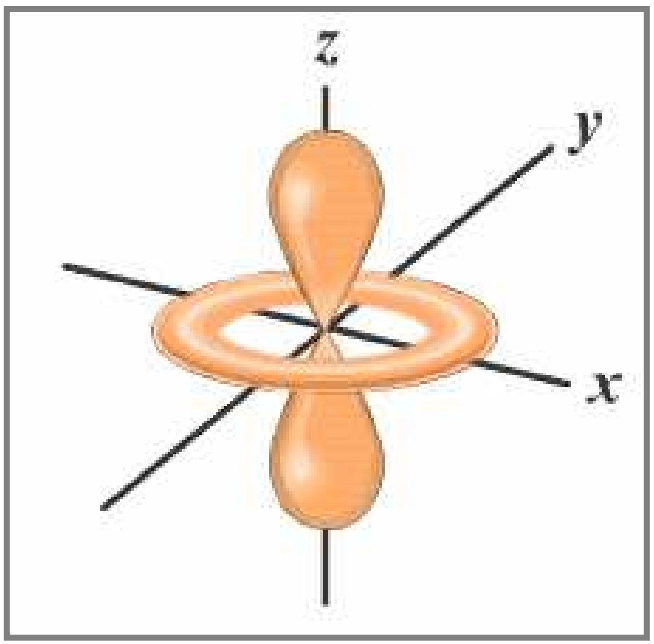

z
y
x

I. Waves and Particles

- De Broglie’s Hypothesis
  - Particles have wave characteristics
  - Waves have particle characteristics
  - $\lambda = h/m\nu$

- Wave-Particle Duality of Nature
- Waves properties are significant at small momentum

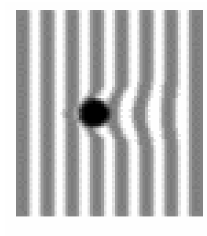
Electrons as Waves

Louis de Broglie
~1924

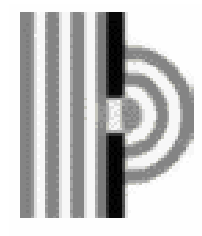
- Louis de Broglie (1924)
  - Applied wave-particle theory to electrons
  - electrons exhibit *wave* properties

QUANTIZED WAVELENGTHS

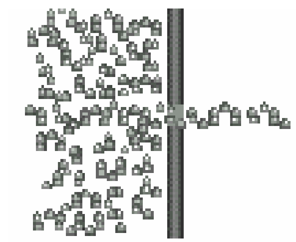
Dual Nature of Light



Waves can bend
around small obstacles…



…and fan out
from pinholes.



Particles *effuse* from pinholes

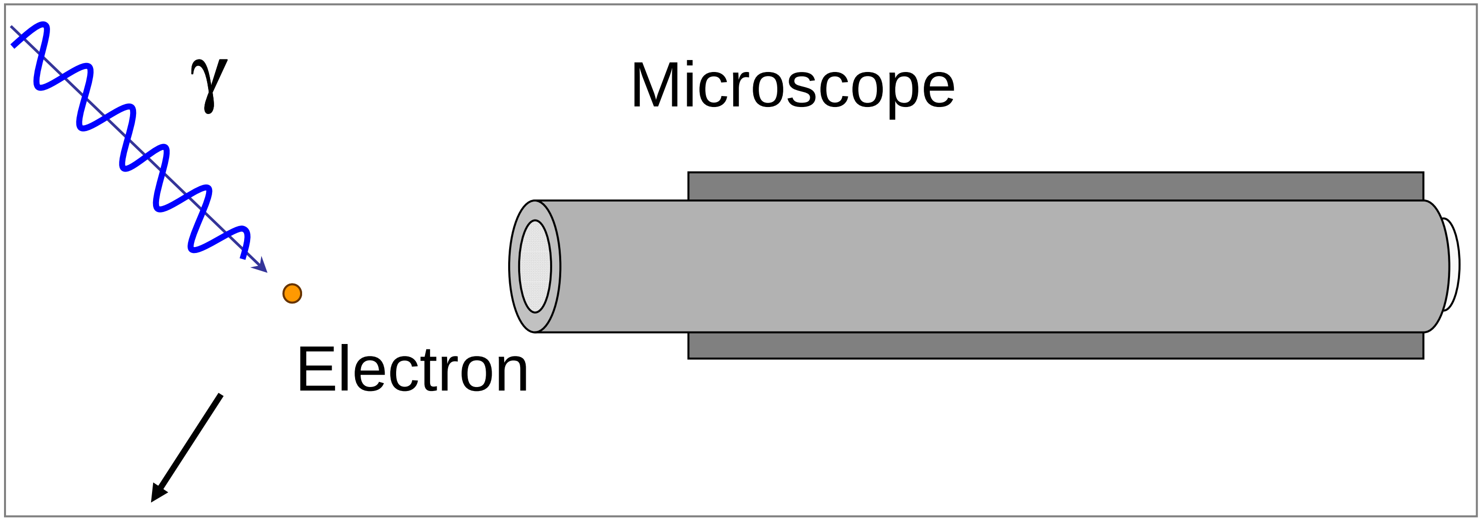
Three ways to tell a wave from a particle…

wave behavior	particle behavior
waves interfere	particle collide
waves diffract	particles effuse
waves are delocalized	particles are localized

Quantum Mechanics

Werner Heisenberg
~1926

- Heisenberg Uncertainty Principle
  – Impossible to know both the *velocity* and *position* of an electron at the same time



Heisenberg uncertainty principle

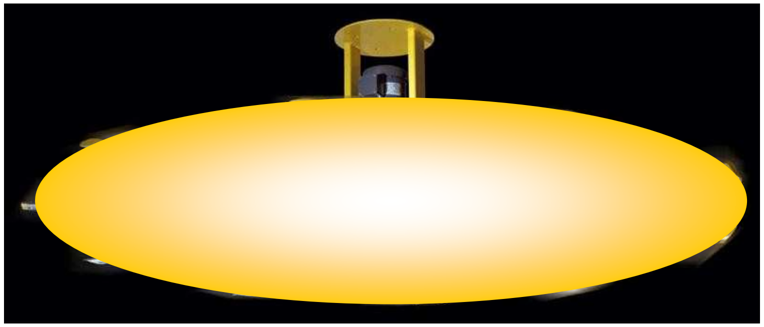
- In order to observe an electron, one would need to hit it with photons having a very short wavelength.
- Short wavelength photons would have a high frequency and a great deal of energy.
- If one were to hit an electron, it would cause the motion and the speed of the electron to change.
- Lower energy photons would have a smaller effect but would not give precise information.

II. The electron as a wave

Schrödinger’s wave equation

– Used to determine the probability of finding the H electron at any given distance from the nucleus

– Electron best described as a cloud
  - Effectively covers all points at the same time (fan blades)



Quantum Mechanics


Erwin Schrödinger
~1926

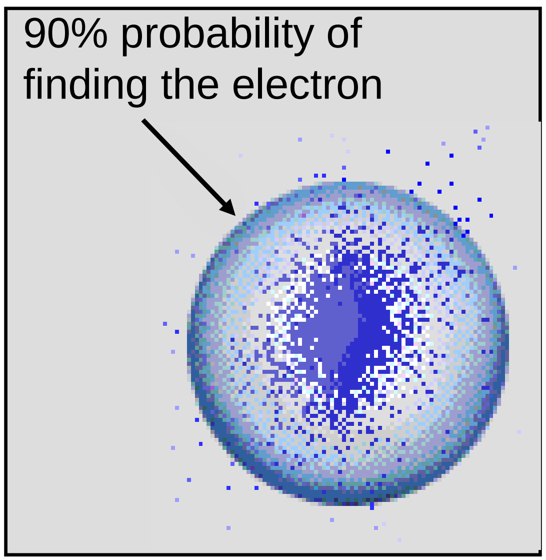
- **Schrödinger Wave Equation** (1926)
  - finite # of solutions ⇒ *quantized* energy levels
  - defines *probability* of finding an electron

$$\Psi_{1s} = \frac{1}{\sqrt{\pi}}\left(\frac{Z}{a_0}\right)^{3/2} e^{-\sigma}$$

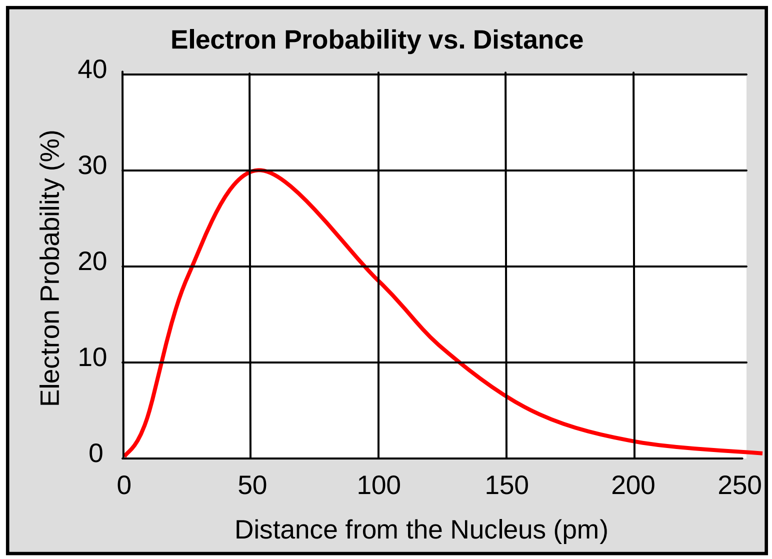
Courtesy Christy Johannesson www.nisd.net/communicationsarts/pages/chem

Quantum Mechanics

- **Orbital** ("electron cloud")
  - Region in space where there is 90% probability of finding an electron



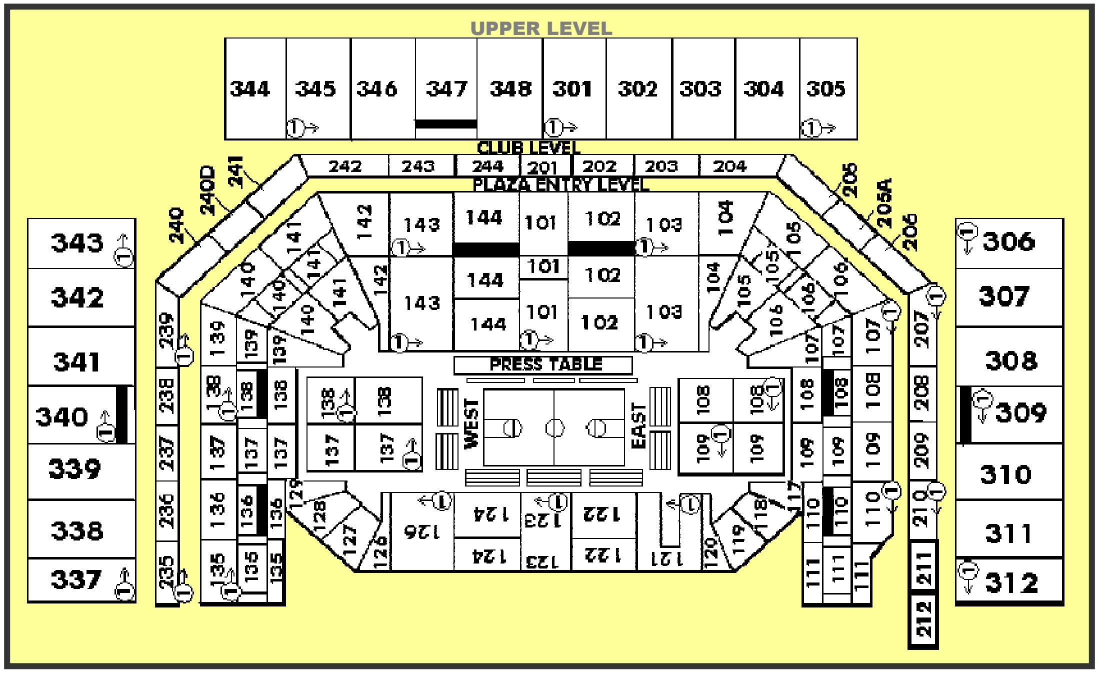
Orbital



Courtesy Christy Johannesson www.nisd.net/communicationsarts/pages/chem

Quantum Numbers

- **Four Quantum Numbers:**
  – Specify the "address" of each electron in an atom



Courtesy Christy Johannesson www.nisd.net/communicationsarts/pages/chem

III. Quantum Numbers

- Used the wave equation to represent different energy states of the electrons
- Set of four #’s to represent the location of the outermost electron
- Here we go…

Quantum Numbers

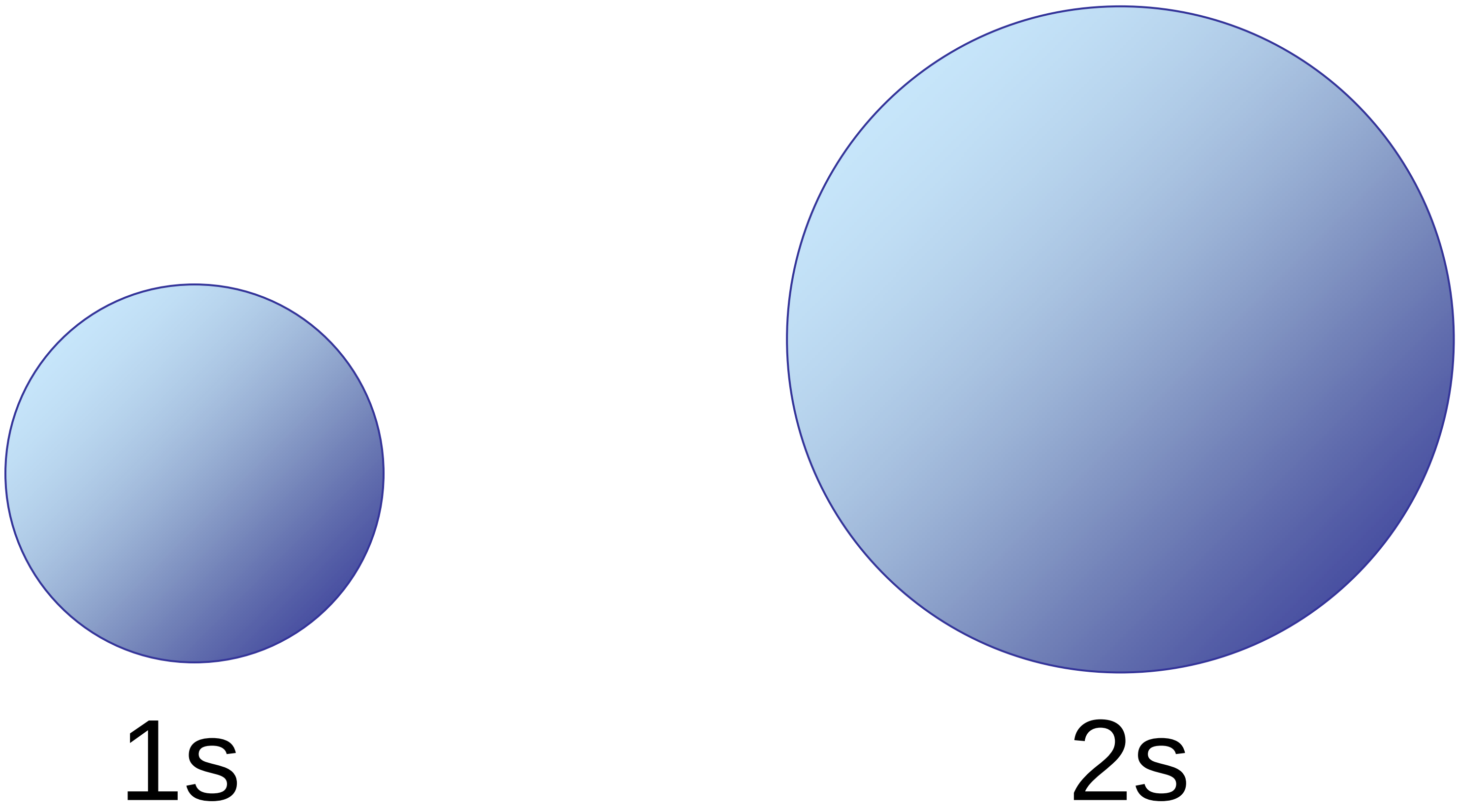
Principal Quantum Number (n)

Angular Momentum Quantum # (l)

Magnetic Quantum Number (m_l)

Spin Quantum Number (m_s)

Relative Sizes 1s and 2s

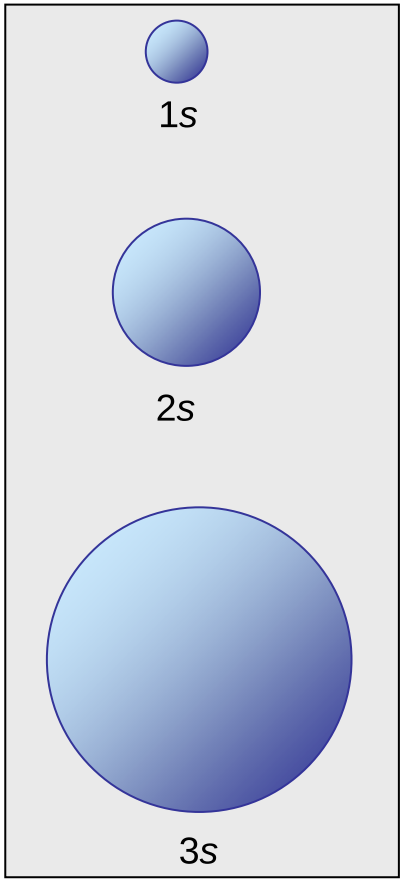


Zumdahl, Zumdahl, DeCoste, World of Chemistry 2002, page 334

Quantum Numbers

1. Principal Quantum Number (*n*)

- Energy level
- Size of the orbital
- n^2 = # of orbitals in the energy level



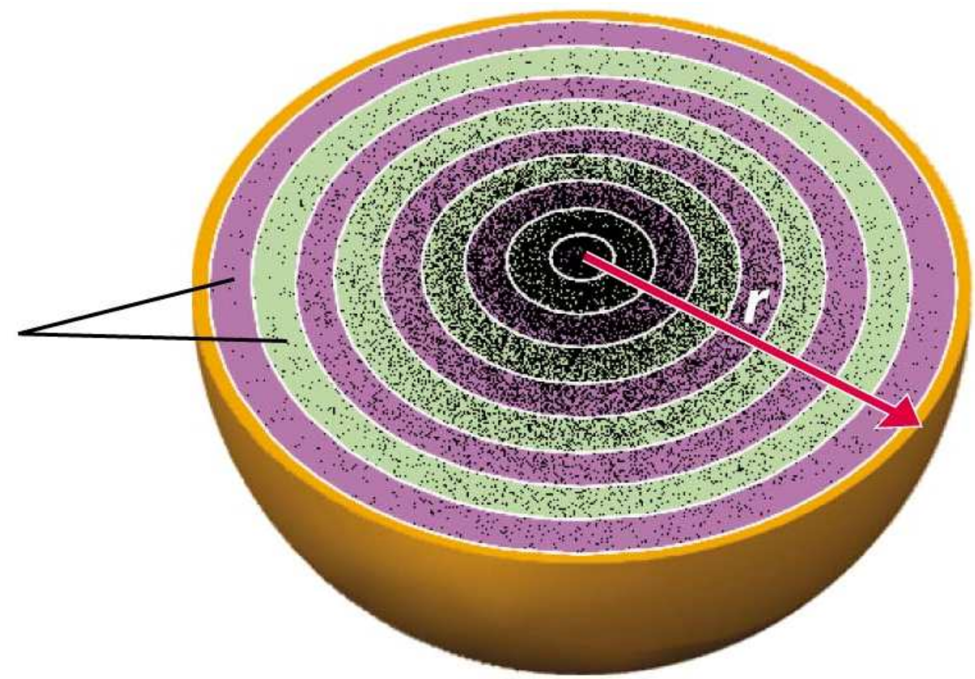
Courtesy Christy Johannesson www.nisd.net/communicationsarts/pages/chem

The Principal quantum number

The quantum number *n* is the principal quantum number.

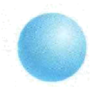
- The principal quantum number tells the average relative distance of the electron from the nucleus
- *n* = 1, 2, 3, 4 . . .
- As *n* increases for a given atom, so does the average distance of the electrons from the nucleus.
- Electrons with higher values of *n* are easier to remove from an atom.
- All wave functions that have the same value of *n* are said to constitute a **principal shell** because those electrons have similar average distances from the nucleus.

1*s* orbital imagined as “onion”

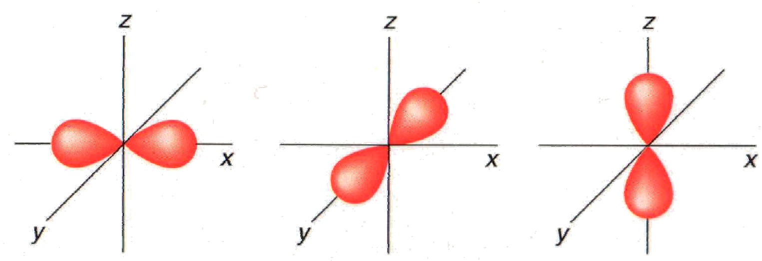


Shapes of s, p, and d-Orbitals

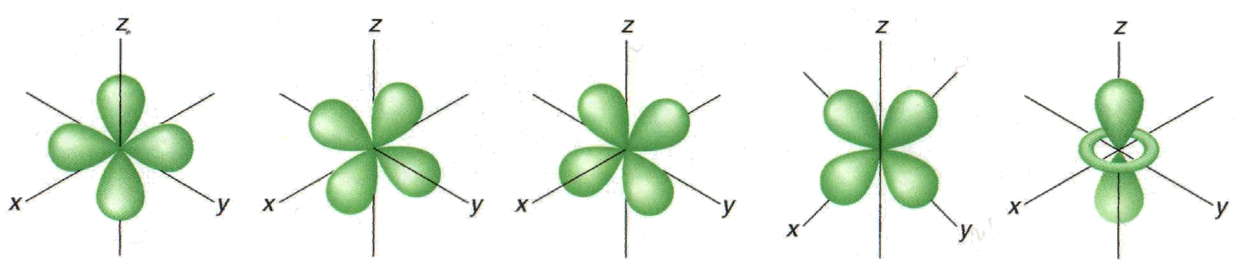
***s* orbital**



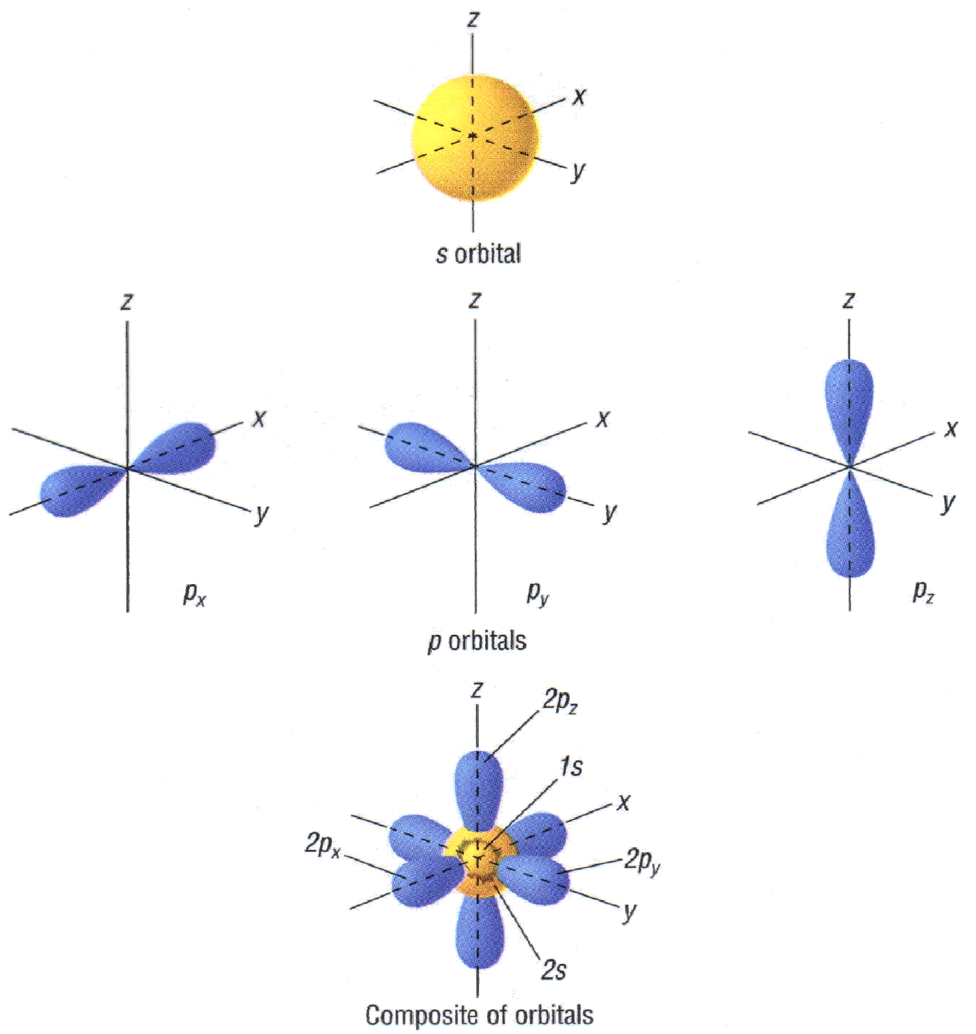
***p* orbitals**



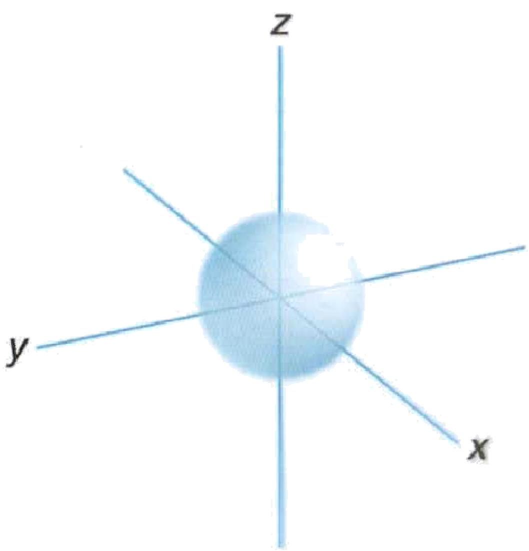
***d* orbitals**



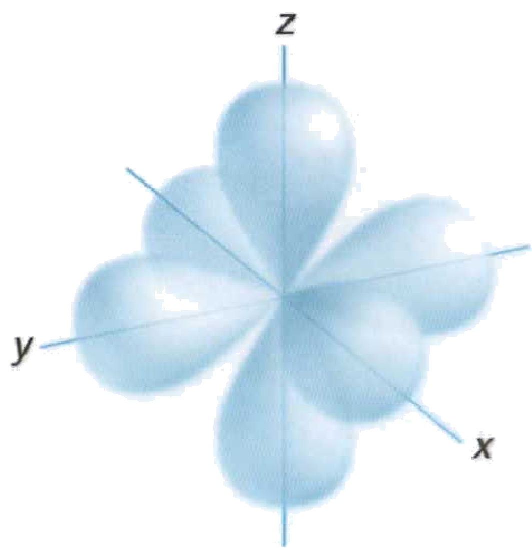
Atomic Orbitals



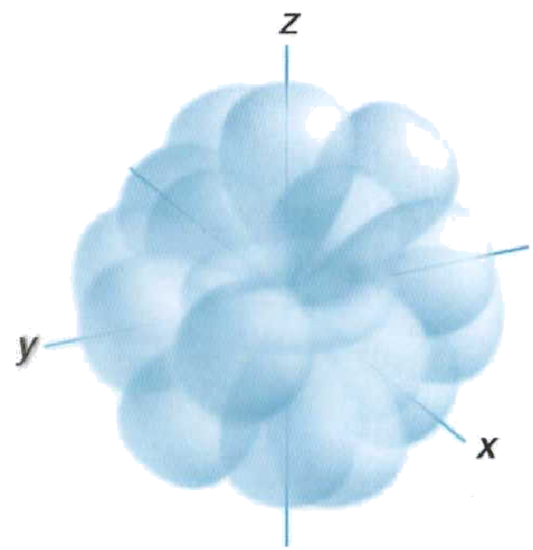
s, p, and d-orbitals



A
s orbitals:
Hold 2 electrons
(outer orbitals of
Groups 1 and 2)

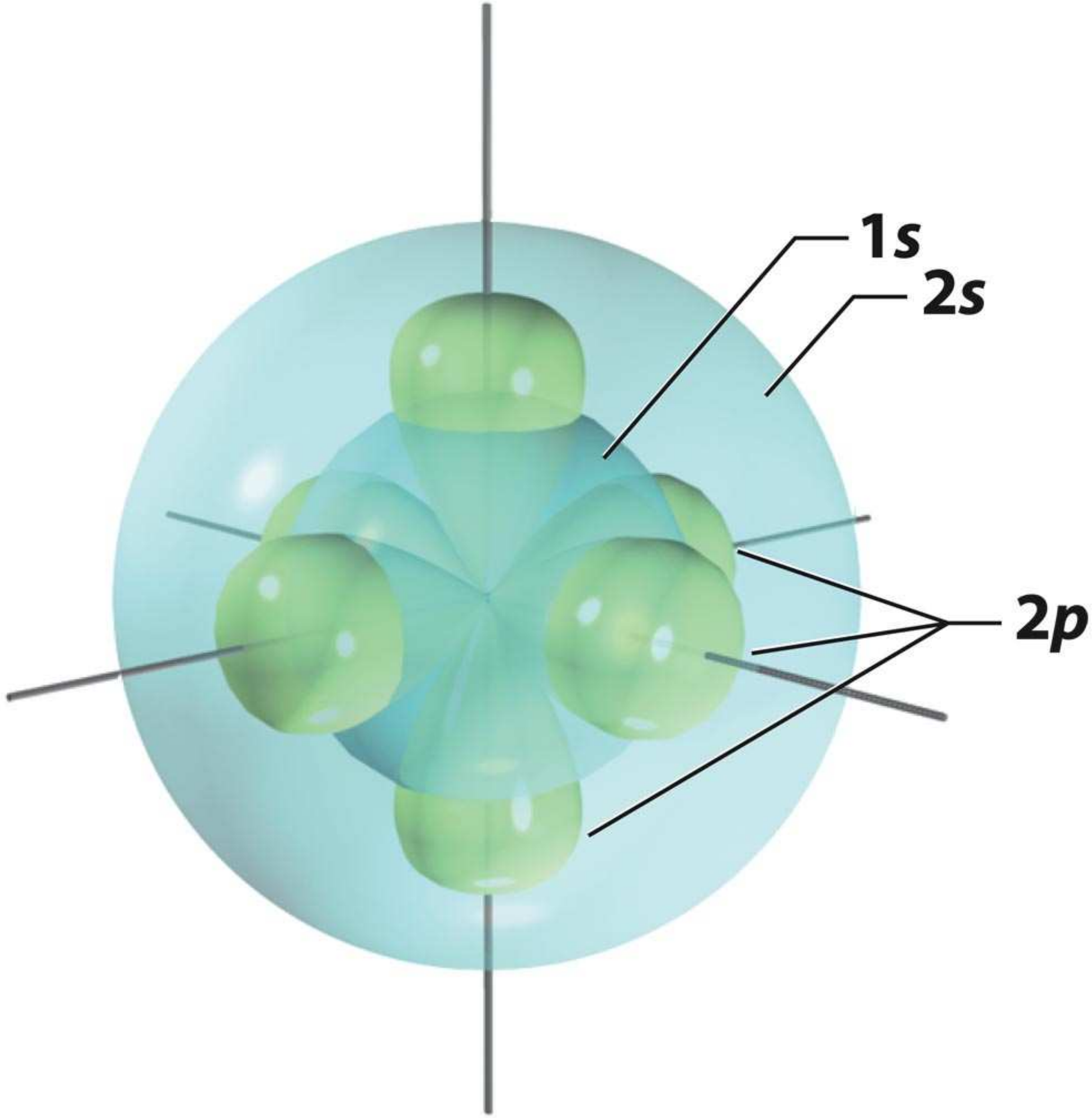


B
p orbitals:
Each of 3 pairs of
lobes holds 2 electrons
= 6 electrons
(outer orbitals of
Groups 13 to 18)

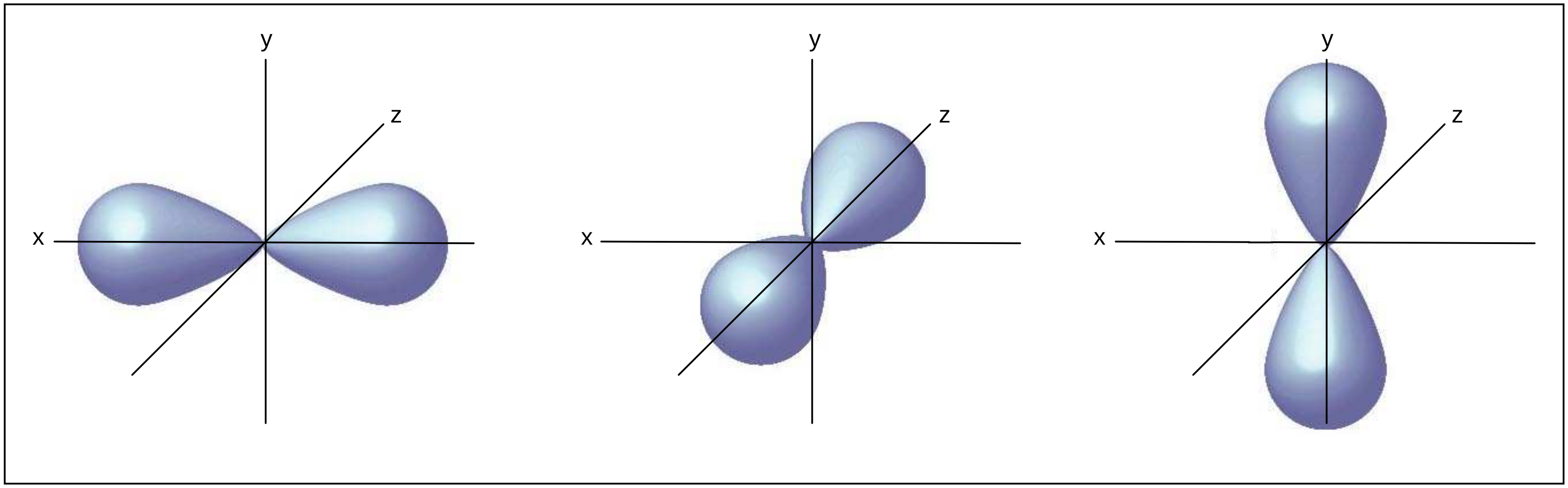


C
d orbitals:
Each of 5 sets of
lobes holds 2 electrons
= 10 electrons
(found in elements
with atomic no. of 21
and higher)

Kelter, Carr, Scott, , Chemistry: A World of Choices 1999, page 82

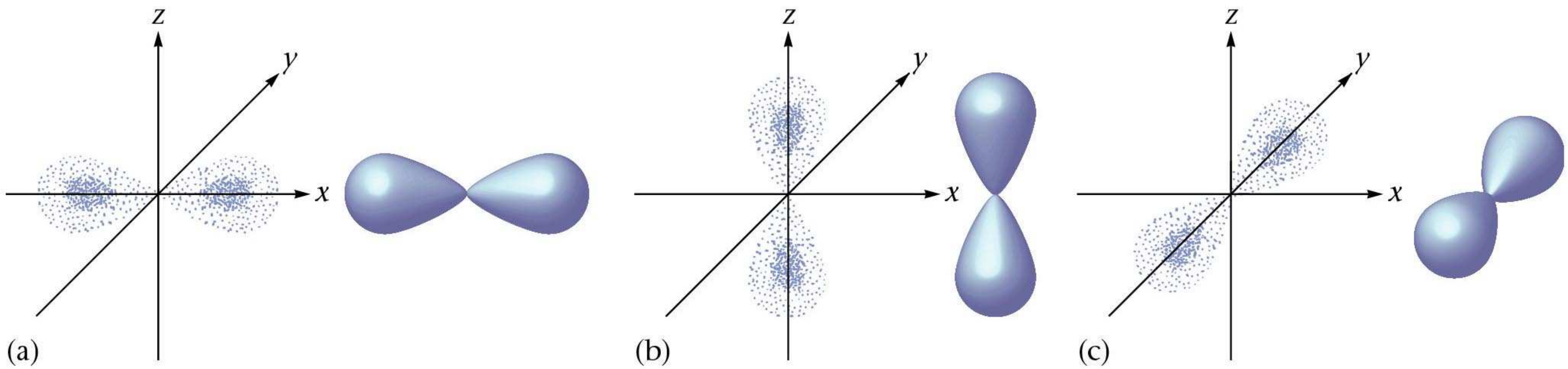

1s
2s
2p

Quantum Numbers



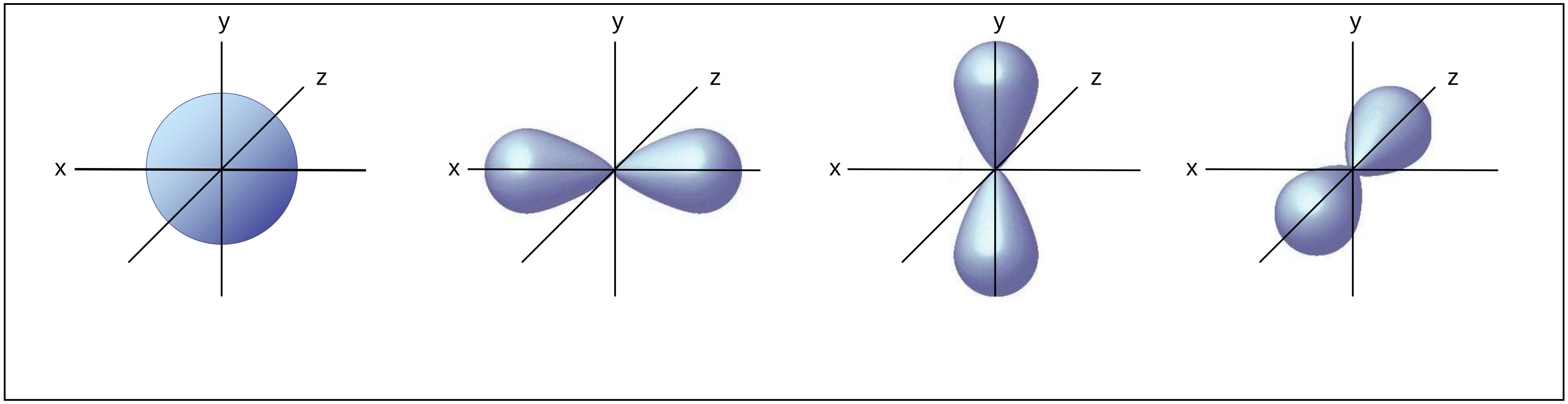
p_x p_z p_y

p-Orbitals

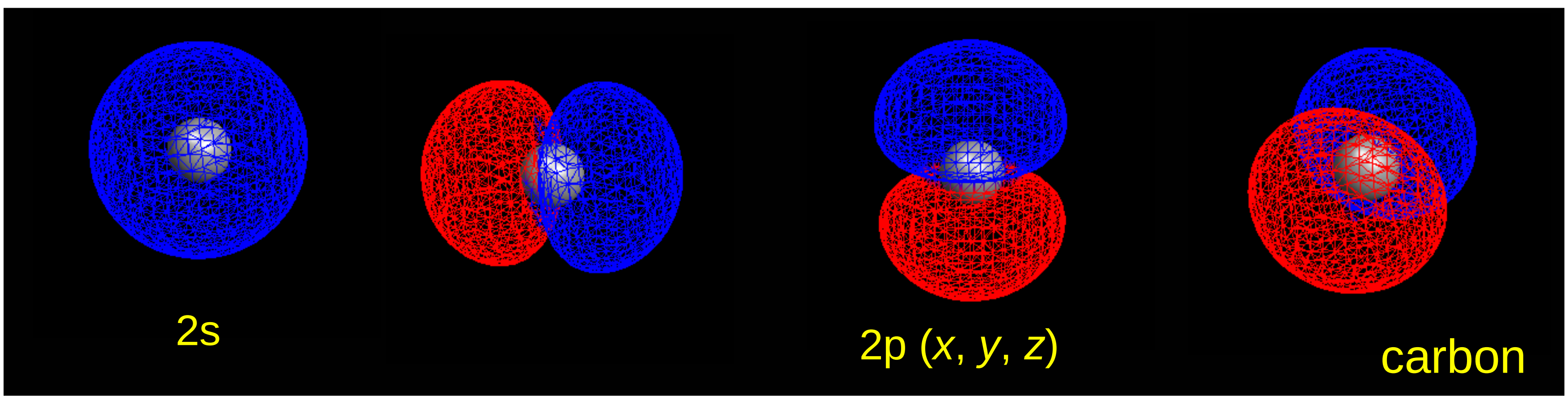


p_x p_z p_y

Zumdahl, Zumdahl, DeCoste, World of Chemistry 2002, page 335



$s \qquad p_x \qquad p_z \qquad p_y$



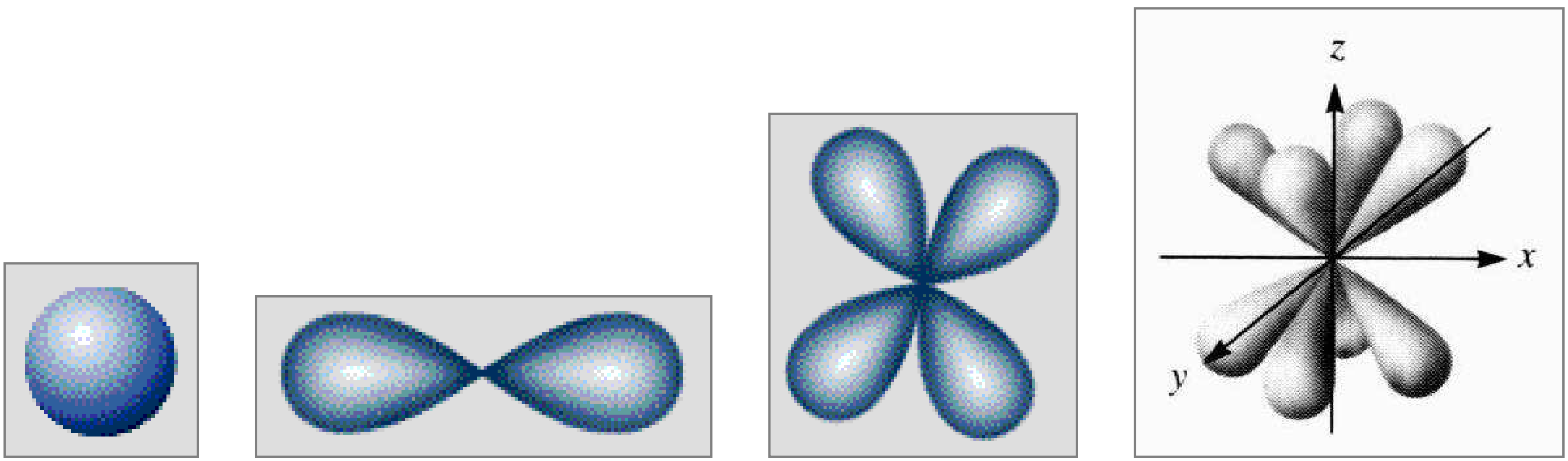
Mark Wirtz, Edward Ehrat, David L. Cedeno*

Quantum Numbers

2. Angular Momentum Quantum # ***(l)***

– Energy sublevel

– Shape of the orbital



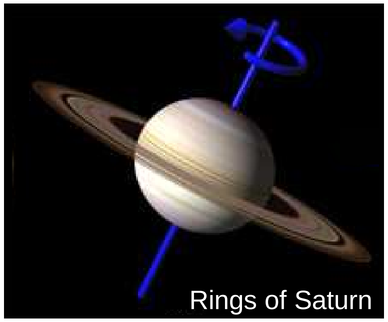
s p d f

Courtesy Christy Johannesson www.nisd.net/communicationsarts/pages/chem

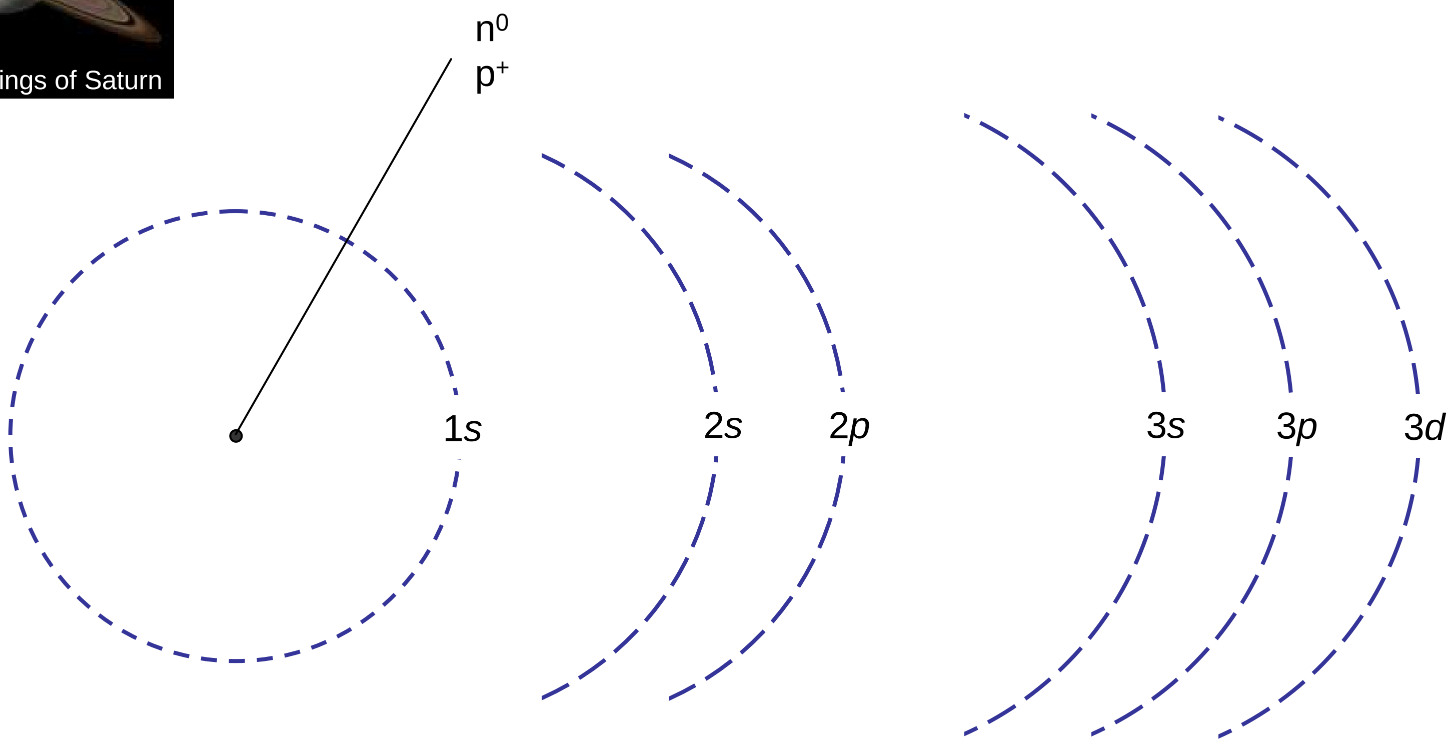
The azimuthal quantum number

Second quantum number *l*
is called the **azimuthal quantum number**

- – Value of *l* describes the *shape* of the region of space occupied by the electron
- – Allowed values of *l* depend on the value of *n* and can range from 0 to *n* – 1
- – All wave functions that have the same value of both *n* and *l* form a **subshell**
- – Regions of space occupied by electrons in the same subshell have the same shape but are oriented differently in space



A Cross Section of an Atom



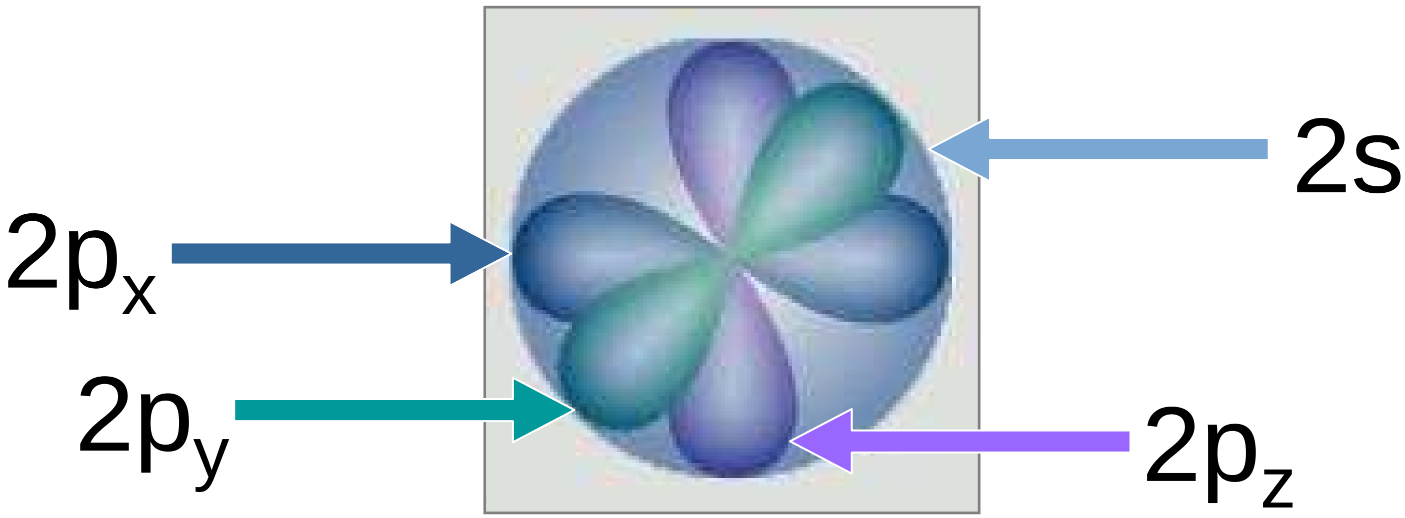
The first ionization energy level has only one sublevel (1s).
The second energy level has two sublevels (2s and 2p).
The third energy level has three sublevels (3s, 3p, and 3d).

Although the diagram suggests that electrons travel in circular orbits, this is a simplification and is *not actually the case*.

Corwin, Introductory Chemistry 2005, page 124

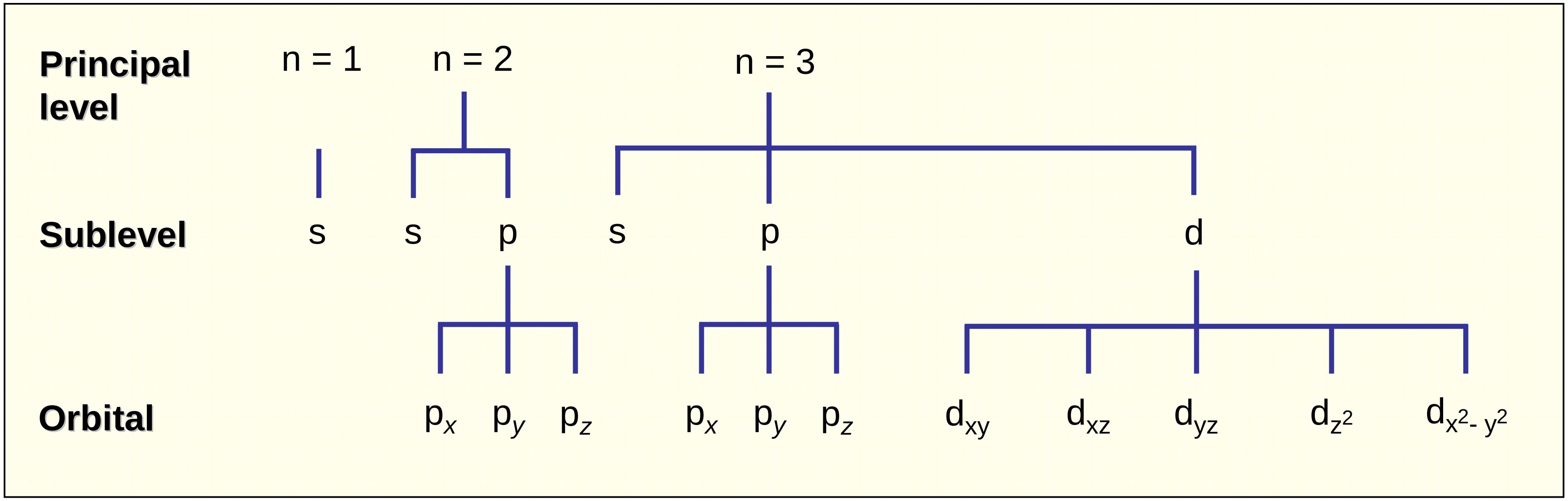
Quantum Numbers

- Orbitals combine to form a spherical shape.



Courtesy Christy Johannesson www.nisd.net/communicationsarts/pages/chem

Quantum Numbers



- n = # of sublevels per level
- n^2 = # of orbitals per level
- Sublevel sets: **1** s, **3** p, **5** d, **7** f

Courtesy Christy Johannesson www.nisd.net/communicationsarts/pages/chem

Maximum Capacities of Subshells and Principal Shells

n	1	2		3			4				...*n*
l	0	0	1	0	1	2	0	1	2	3	
Subshell designation	*s*	*s*	*p*	*s*	*p*	*d*	*s*	*p*	*d*	*f*	
Orbitals in subshell	1	1	3	1	3	5	1	3	5	7	
Subshell capacity	2	2	6	2	6	10	2	6	10	14	
Principal shell capacity	2	8		18			32				...$2n^2$

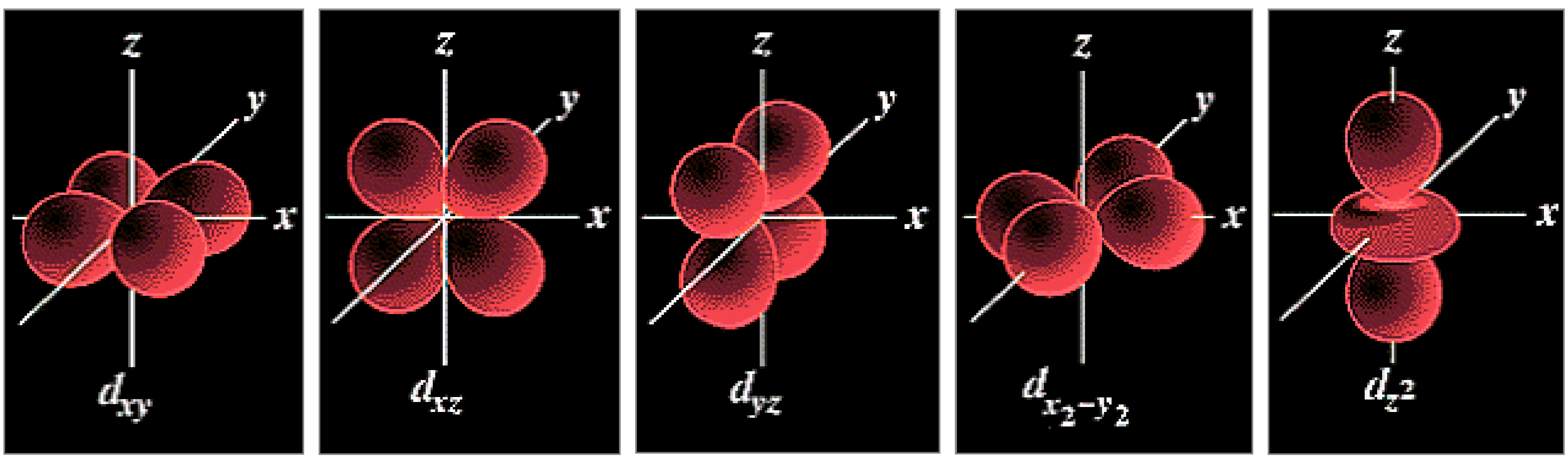
Hill, Petrucci, General Chemistry *An Integrated Approach* 1999, page 320

Quantum Numbers

3. Magnetic Quantum Number (m_l)

– Orientation of orbital

– Specifies the exact orbital within each sublevel



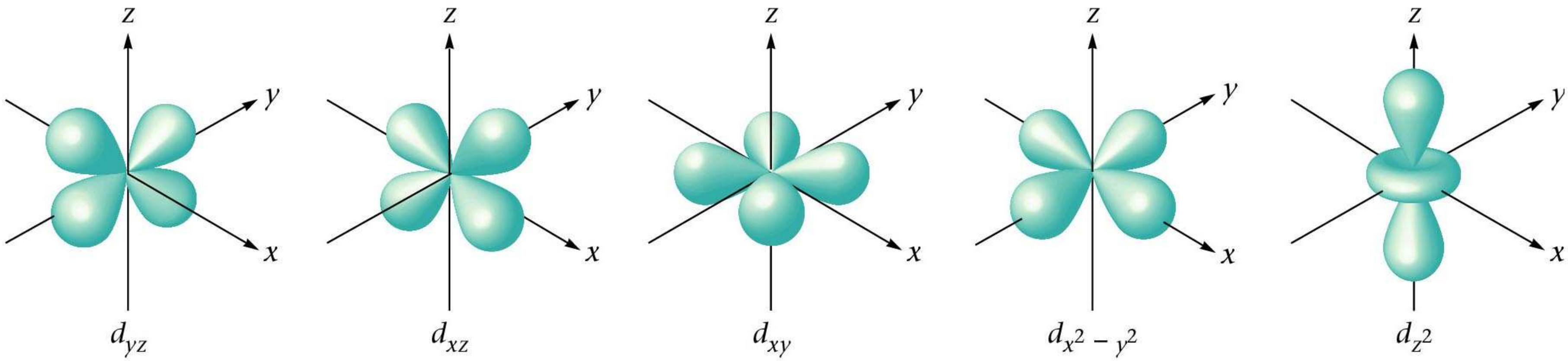
Courtesy Christy Johannesson www.nisd.net/communicationsarts/pages/chem

The magnetic quantum number

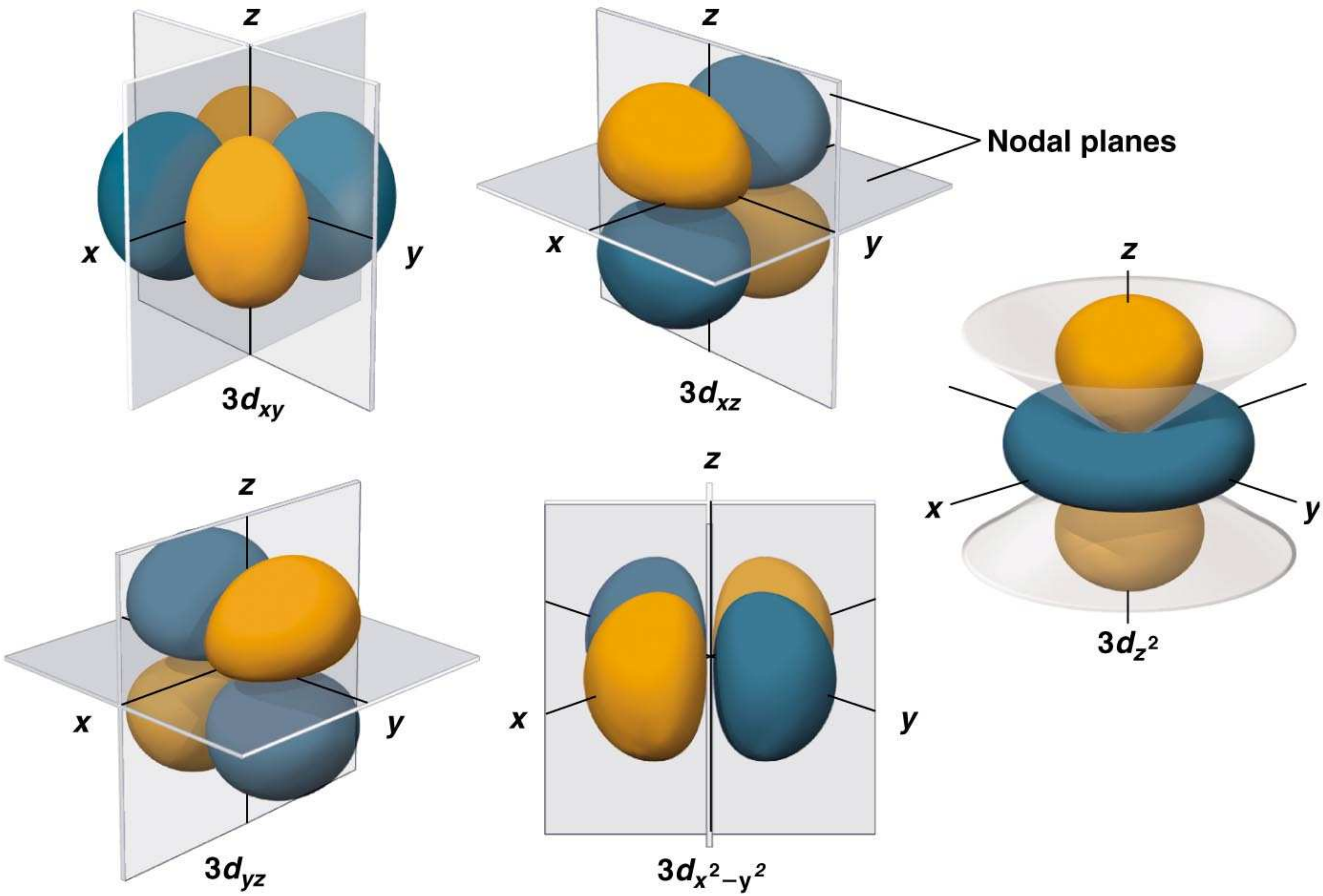
Third quantum is m_l, the **magnetic quantum number**

- Value of m_l describes the *orientation* of the region in space occupied by the electrons with respect to an applied magnetic field
- Allowed values of m_l depend on the value of l
- m_l can range from $-l$ to l in integral steps
  $m_l = -l, -l + 1, \ldots 0 \ldots, l - 1, l$
- Each wave function with an allowed combination of n, l, and m_l values describes an **atomic orbital**, a particular spatial distribution for an electron
- For a given set of quantum numbers, each principal shell contains a fixed number of subshells, and each subshell contains a fixed number of orbitals

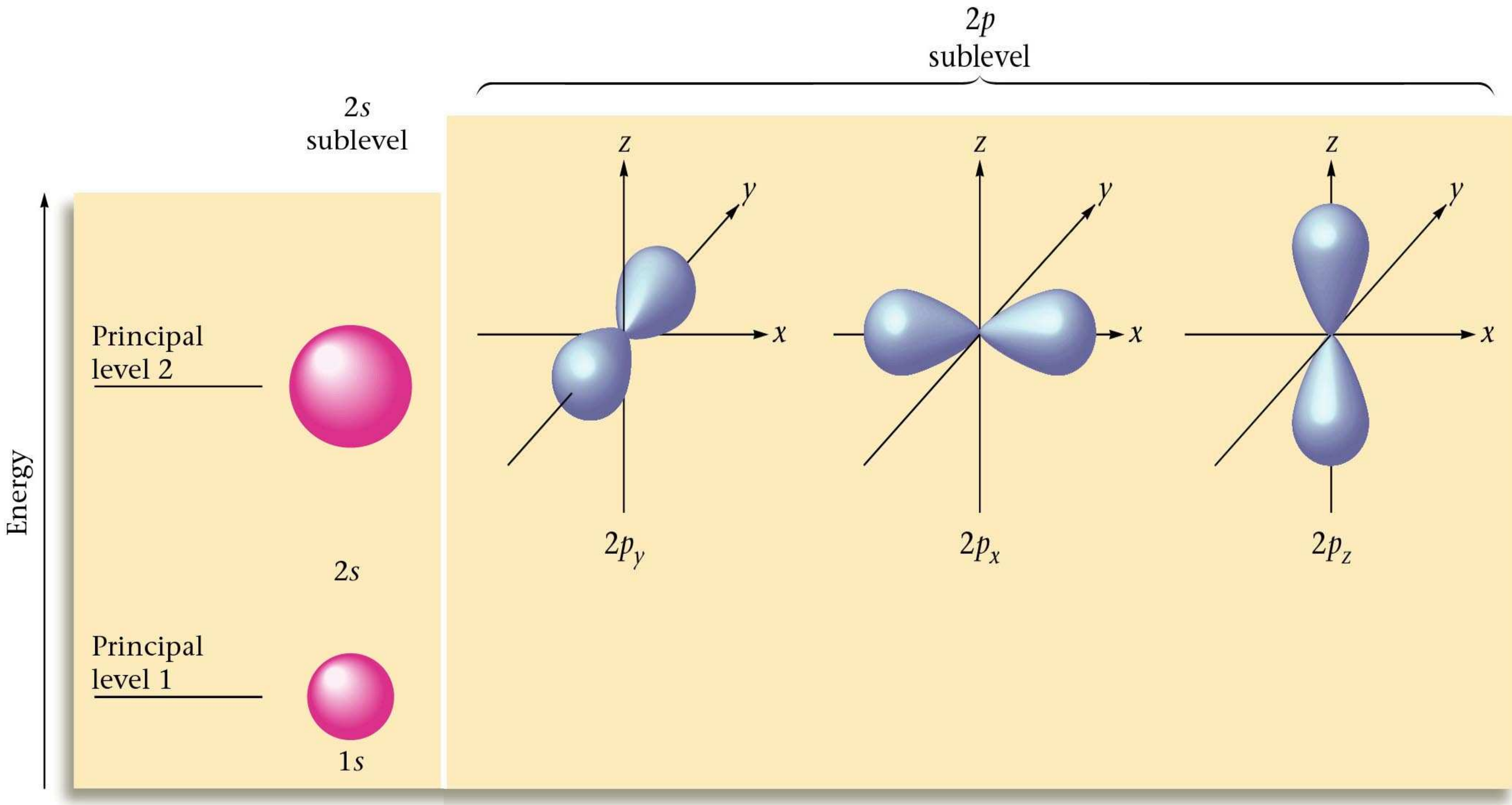
d-orbitals



Zumdahl, Zumdahl, DeCoste, World of Chemistry 2002, page 336


z
x
y
3d_{xy}
z
x
y
3d_{xz}
Nodal planes
z
x
y
3d_{z^2}
z
x
y
3d_{yz}
z
x
y
3$d_{x^2-y^2}$

Principal Energy Levels 1 and 2

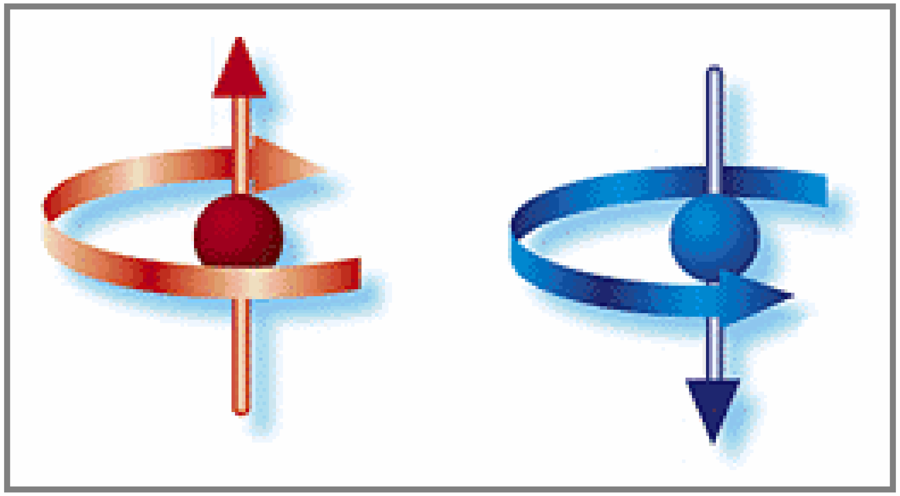


Quantum Numbers

4. Spin Quantum Number ***(m_s)***

– Electron spin ⇒ +½ or -½

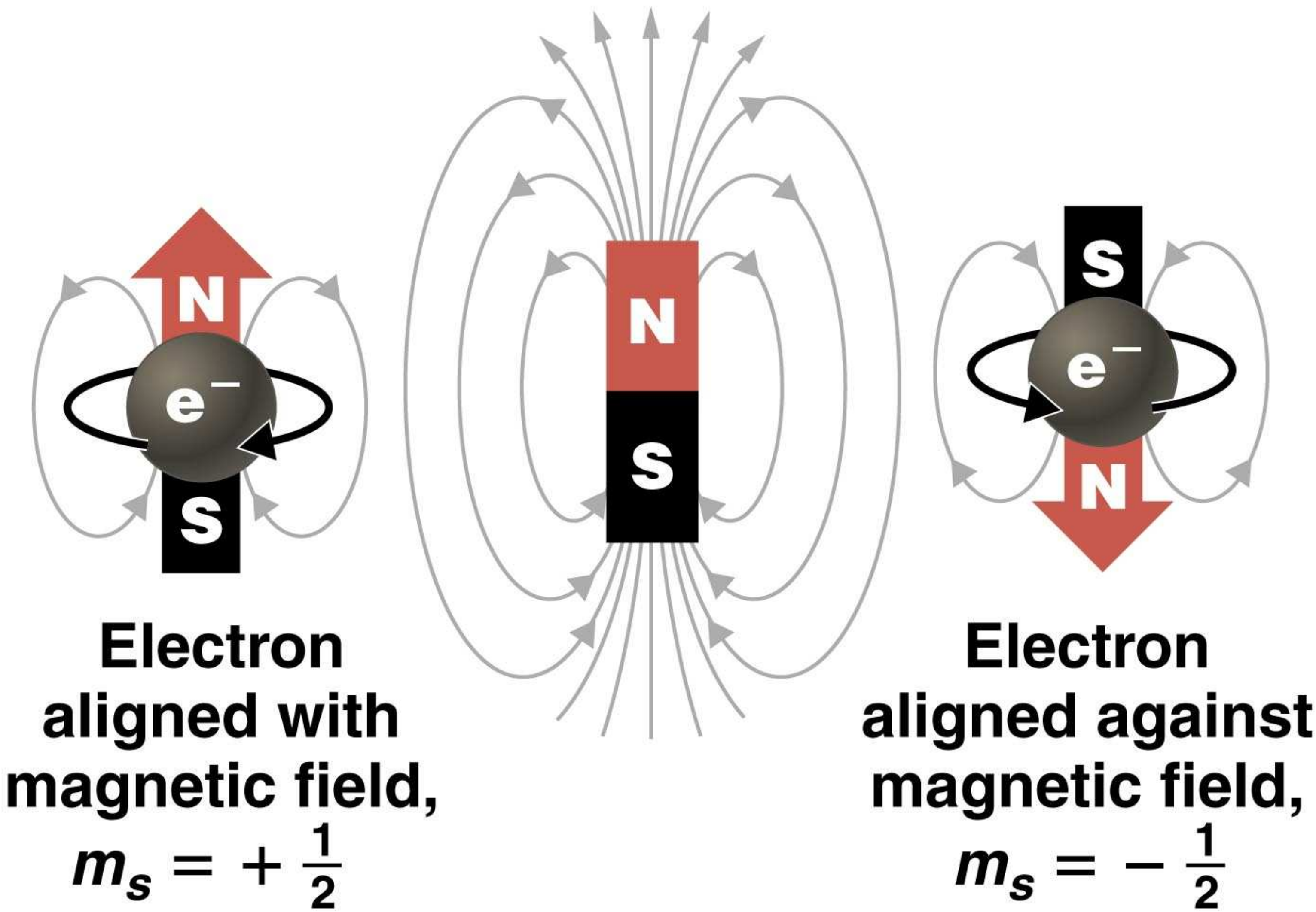
– An orbital can hold 2 electrons that spin in opposite directions.



Courtesy Christy Johannesson www.nisd.net/communicationsarts/pages/chem

Electron Spin: The Fourth Quantum Number

- When an electrically charged object spins, it produces a magnetic moment parallel to the axis of rotation and behaves like a magnet.
- A magnetic moment is called ***electron spin.***
- An electron has two possible orientations in an external magnetic field, which are described by a fourth quantum number $\boldsymbol{m_s}$.
- For any electron, m_s can have only two possible values, designated + (up) and – (down), indicating that the two orientations are opposite and the subscript *s* is for spin.
- An electron behaves like a magnet that has one of two possible orientations, aligned either with the magnetic field or against it.


N
e⁻
S
Electron aligned with magnetic field,
$m_s = +\frac{1}{2}$
N
S
S
e⁻
N
Electron aligned against magnetic field,
$m_s = -\frac{1}{2}$

Quantum Numbers

Wolfgang Pauli

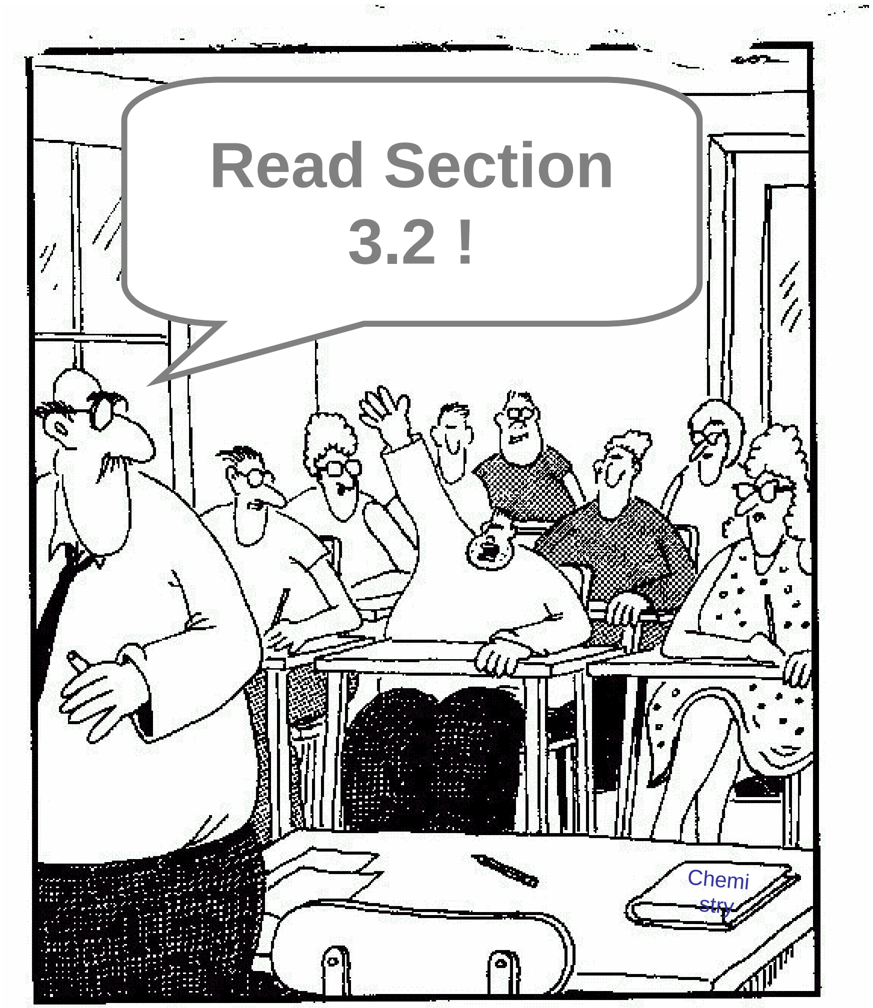
- Pauli Exclusion Principle
  - No two electrons in an atom can have the same 4 quantum numbers.
  - Each electron has a unique “address”:

1. Principal # → energy level
2. Ang. Mom. # → sublevel *(s,p,d,f)*
3. Magnetic # → orbital
4. Spin # → electron

Allowed Sets of Quantum Numbers for Electrons in Atoms

Level n	**1**	**2**				**3**								
Sublevel l	0	0	1			0	1			2				
Orbital $\mathbf{m}_l$	0	0	1	0	-1	0	1	0	-1	2	1	0	-1	-2
Spin $\mathbf{m}_s$ $\uparrow$ = +1/2 $\downarrow$ = -1/2	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$

Feeling overwhelmed?



"Teacher, may I be excused? My brain is full."

Courtesy Christy Johannesson www.nisd.net/communicationsarts/pages/chem

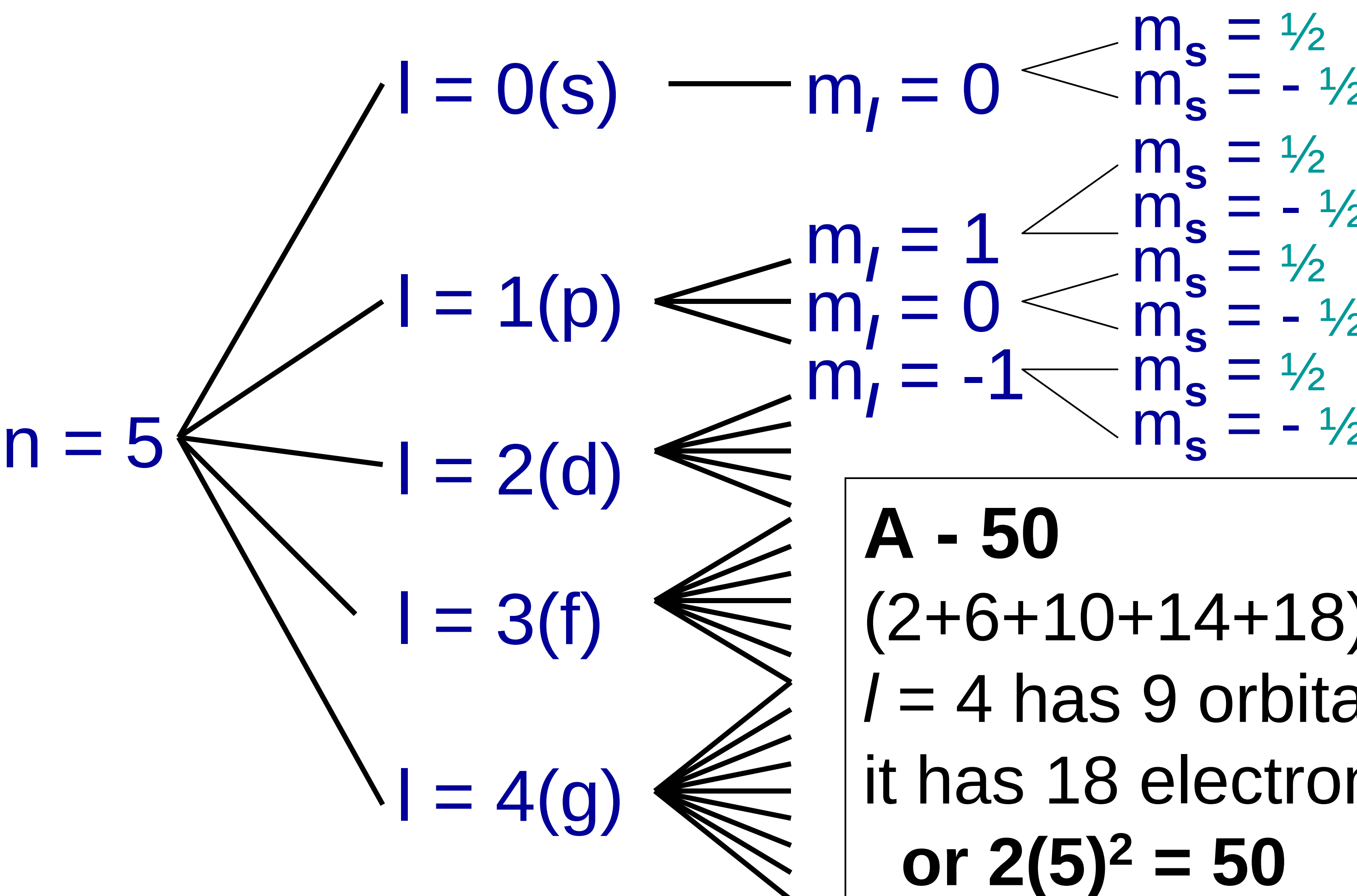
Quantum Numbers

n	$\longrightarrow$	shell	1, 2, 3, 4, ...
l	$\longrightarrow$	subshell	0, 1, 2, ... n - 1
m_l	$\longrightarrow$	orbital	$- l$ ... 0 ... $+l$
m_s	$\longrightarrow$	electron spin	$+{}^{1}/_{2}$ and $-{}^{1}/_{2}$

Electrons in n = 5 shell

What is the maximum shell population of n = 5?

½



A - 50

(2+6+10+14+18)

l = 4 has 9 orbitals:

it has 18 electrons

or $2(5)^2 = 50$